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The research in infrared astronomy has modeled several classes of infrared sources and modified and generalized existing computer codes. The effects of temperature fluctuations due to small grains on the energy spectrum and infrared surface brightness of interstellar clouds heated externally by the interstellar radiation field were studied. A detailed study has begun on the grain formation problem in stellar outflows. The effects of fractal dust grains on the spectrum of infrared sources has been studied. Models are being developed of the physical conditions in the circumstellar envelopes of evolved stars. The chemistry of two dense interstellar clouds is being studied. The effect of temperature dependent opacity on the emergent spectra of infrared sources is being investigated.

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PI: Chun Ming Leung
Institution: Rensselaer Polytechnic Institute
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Narrative:

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PM: H.R.Radoski

Rensselaer

December 6, 1991

Dr. Henry R. Radoski, Director
Space Physics Program
Life Sciences Division
Air Force Office of Scientific Research
AFOSR/NP, Building 410
Bolling Air Force Base, D. C. 20332-6448

Re.: 1990-91 Research Progress Report (Grant AFOSR-89-0104)

Dear Dr. Radoski:

Thank you for your recent approval of a six-month no-cost extension of my AFOSR grant supporting the project: "*Probing Cosmic Infrared Sources: a Computer Modeling Approach*". As you suggested, in lieu of a lengthy third annual technical report, I am submitting a brief summary of the research activities in the past twelve months. A detailed final technical report will be submitted after the expiration of this grant on April 30, 1992, as required.

Personnel:
At present the research group working on this project consists of 6 people: Chun M. Leung (PI), Michael P. Egan, Steven D. Doty, Michael E. Fogel, Monika E. Kress and Curtis Potterveld (all graduate students). Both Egan and Doty are Ph. D. candidates. The two postdoctoral fellows, Drs. Steven B. Charnley and K. N. Nagendra, completed their terms of appointments and left to take up positions elsewhere: Charnley is now at the NASA Ames Research Center while Nagendra is at the Indian Institute of Astrophysics at Bangalore in India. In addition, three undergraduates were involved in research this past summer.

Research:
The research effort has gone into modifying and generalizing existing computer codes as well as in the modeling of several classes of infrared sources.

(1) We continued to study the effects of temperature fluctuations due to small grains on the energy spectrum and infrared surface brightness of interstellar clouds heated externally by the interstellar radiation field. Radiation transport models with conventional large grains, very small grains, and polycyclic aromatic hydrocarbons (PAHs) are constructed. Applying the model results to the IRAS observations of the diffuse cloud in Chamaeleon, it is found that the 25 μm emission is most likely due to small grains which also contribute significantly to the observed 12 μm emission. However, the majority of the 12 μm flux is due to PAHs. The emission at 60 and 100 μm is mostly due to large grains (with radius $\sim 0.1\ \mu$m) heated under equilibrium conditions. Furthermore, to produce the observed limb-brightening at various infrared wavelengths, the spatial distribution of the small grains and PAHs must be more extended than the large grains.

(2) We have begun a detailed study of the grain formation problem in stellar outflows. Grain formation consists of nucleation followed by growth. Most studies have used classical nucleation theory to describe the formation rate of grain nuclei in a supersaturated vapor, under the assumption of local thermodynamic equilibrium. However, the nucleation process is best determined by solving a system of kinetic

equations. The growth of the nuclei is then determined by solving a set of moment equations which are highly dependent on the nucleation rate of particles in the gas. To test the validity of classical nucleation theory in astrophysical environments, a truncated set of kinetic equations is solved simultaneously with the moment equations, thus allowing a self-consistent treatment of grain nucleation and growth. It is found that classical nucleation theory allows nucleation of grains to occur at a much lower supersaturation than is calculated from the kinetic equations, thus predicting dust formation too near a star, overestimating the number of dust grains produced , and underestimating the average grain size. The effect of these results on radiative transfer in the dust shell is being investigated.

(3) We have studied the effects of fractal dust grains on the spectrum of infrared sources by considering non-spherical dust grains produced by two fractal growth processes: particle-by-particle aggregation or cluster-by-cluster aggregation. By approximating a fractal grain as a collection of dipoles, the discrete dipole approximation is used to calculate the grain opacity. Optical constants for both bulk material and amorphous clusters are utilized. Using these dust opacities for fractal grains, radiation transport models of infrared sources are constructed to study the effect of grain size, shape, and composition on the IR spectrum. It is found that, compared to models with spherical grains of the same composition and volume, models with fractal carbon grains show a shift in the peak flux toward longer wavelengths. The less compact fractal dust grains tend to be cooler than spherical grains. These differences are due to a higher ratio of geometrical cross section to volume for fractal grains. For fractal grains with the same ratio the overall grain shape plays only a minor role.

(4) We have begun a study to model in detail the physics and chemistry of the circumstellar envelopes of evolved stars. The goal is to develop a comprehensive model in which both chemical evolution and radiation hydrodynamics are treated self-consistently. As an example, the effect of shielding of the ambient interstellar radiation by dust and self-shielding of H_2 and CO on the photoionization rates are considered by solving the radiation transport problem accurately. Model results will be compared with available observations of evolved stars.

(5) We have begun a study to understand the chemistry of the two dense interstellar clouds, L134N and TMC-1. These clouds have similar physical conditions but display remarkable differences in chemical abundances. In particular, whereas TMC-1 exhibits relatively large abundances of many complex, unsaturated, carbon-rich species, L134N appears to have larger abundances of some oxygen-rich species as well as saturated simple molecules. This discrepancy may be due to a difference in the initial gas-phase [C]/[O] ratio or due to the clouds being in different stages of evolution. To delineate the effects of different initial composition versus cloud evolution, the chemical model of Herbst and Leung are used to study the chemical evolution of these two clouds. In the models the original reaction network has been expanded to include 3517 reactions involving 385 species. It is found that certain molecules may prove to be particularly sensitive probes of the initial [C]/[O] ratio and/or the evolutionary phase of the cloud. In particular, the ratio [NO]/[CO] can be used to differentiate between whether an initial high [C]/[O] ratio (relative to the cosmic value) is due to carbon enrichment or to oxygen depletion, e.g., [NO]/[CO] > 1 for carbon enrichment while [NO]/[CO] < 1 for oxygen depletion.

(6) We have begun to study the effect of temperature-dependent opacity on the emergent spectra of infrared sources. Laboratory evidence indicates that optical constants of grain material depend on the grain temperature. Radiation transport models are constructed in which the dust opacity is allowed to vary with grain temperature. It is found that a temperature-dependent dust opacity affects both the equilibrium grain temperature and the emergent spectrum. The effect is most pronounced on the detailed shape of spectral features. Models are being constructed to study the effects on the intensity and shape of the 10 μm and 20 μm features of silicate grains.

Preliminary results of the research in (2), (3), and (5) will be presented as three poster papers in the upcoming meeting of the American Astronomical Society in Atlanta.

I greatly appreciate the support by AFOSR of this research program. I hope you have received my recent proposal entitled "*Computer Modeling Studies of the Infrared Celestial Backgrounds*" for the DoD program of Augmentation Awards for Science and Engineering Research Training and that the proposal will receive favorable consideration.

Sincerely,

Chun Ming Leung

Chun Ming Leung
Professor of Physics